THE THE LAND

4

OFFICE OF NAVAL RESEARCH

Contract N00014-86-K-0043

TECHNICAL REPORT No. 106

Dwell Time and Average Local Speed in a Resonant Tunneling Structure

by

L. N. Pandey, D. Sahu and Thomas F. George

Prepared for Publication

in

Solid State Communications

Departments of Chemistry and Physics State University of New York at Buffalo Buffalo, New York 14260

July 1989

Reproduction in whole or in part is permitted for any purpose of the United States Government.

This document has been approved for public release and sale; its distribution is unlimited.



REPORT DOCUMENTATION PAGE					Form Approved OMB No. 0704-0188		
1a. REPORT SECURITY CLASSIFICATION Unclassified		16. RESTRICTIVE MARKINGS					
2a. SECURITY CLASSIFICATION AUTHORITY		3. DISTRIBUTION	/AVAILABILITY O	F REPORT			
2b. DECLASSIFICATION / DOWNGRADING SCHEDULE		Approved for public release; distribution unlimited					
4. PERFORMING ORGANIZATION REPORT NUMBE	R(S)	5. MONITORING ORGANIZATION REPORT NUMBER(S)					
UBUFFALO/DC/89/TR-106	5						
6a. NAME OF PERFORMING ORGANIZATION Depts. Chemistry & Physics State University of New York	6b. OFFICE SYMBOL (If applicable)	7a. NAME OF MO	ONITORING ORGA	NIZATION			
State University of New York 6c. ADDRESS (City, State, and ZIP Code) Fronczak Hall, Amherst Campus Buffalo, New York 14260		7b. ADDRESS(City, State, and ZIP Code) Chemistry Program 800 N. Quincy Street Arlington, Virginia 22217					
8a. NAME OF FUNDING/SPONSORING ORGANIZATION Office of Naval Research	8b. OFFICE SYMBOL (If applicable)	9. PROCUREMENT INSTRUMENT IDENTIFICATION NUMBER Contract N00014-86-K-0043					
8c. ADDRESS (City, State, and ZIP Code)		10. SOURCE OF F	UNDING NUMBER	S			
Chemistry Program 800 N. Quincy Street Arlington, Virginia 22217		PROGRAM ELEMENT NO.	PROJECT NO.	TASK NO	WORK UNIT ACCESSION NO.		
11. TITLE (Include Security Classification) Dwell Time and Average I	ocal Speed in a	Resonant Tu	nneling Str	ucture			
12. PERSONAL AUTHOR(S) L. N. Pandey,	D. Sahu and Th	omas F. Geor	ge				
13a. TYPE OF REPORT 13b. TIME CO	OVERED TO	14. DATE OF REPO	RT (Year, Month, y 1989	Day) 15.	PAGE COUNT 16		
16. SUPPLEMENTARY NOTATION Prepared for publication	ition in Solid S	tate Communi	cations				
17. COSATI CODES FIELD GROUP SUB-GROUP	18. SUBJECT TERMS (RESONANT TUNNE DIODE DWELL TIME	S (Continue on reverse if necessary and identify by block number) NELING LOCAL SPEED INTERFACES MICROSCOPIC CALCULATION			EED ES		
19. ABSTRACT (Continue on reverse if necessary		umber)	/	TOROBOO	110 CALCOLATIONS		
We show that the dwell times and the average local speeds of an electron in a resonant tunneling structure depend sensitively on the matching parameter at the interfaces. We point out that there is a need to carry out microscopic calculations to find out which matching parameter is appropriate for a given structure.							
20. DISTRIBUTION / AVAILABILITY OF ABSTRACT UNCLASSIFIED/UNLIMITED SAME AS R	PT. DTIC USERS	21. ABSTRACT SEC	CURITY CLASSIFIC				
22a. NAME OF RESPONSIBLE INDIVIDUAL		226. TELEPHONE (I) 22c. OF	FICE SYMBOL		
DD Form 1473, JUN 86	Previous editions are	(202) 696-4		CI ASSIFICA	TION OF THIS PAGE		

Solid State Communications, in press

DWELL TIME AND AVERAGE LOCAL SPEED IN A RESONANT TUNNELING STRUCTURE

L. N. Pandey, D. Sahu and Thomas F. George
Departments of Physics and Chemistry
Center for Electronic and Electro-optic Materials
239 Fronczak Hall
State University of New York at Buffalo, Buffalo, New York 14260

(Received June 1989 by M. F. Collins)

We show that the dwell times and the average local speeds of an electron in a resonant tunneling structure depend sensitively on the matching parameter at the interfaces. We point out that there is a need to carry out microscopic calculations to find out which matching parameter is appropriate for a given structure.

Recently resonant tunneling diodes (RTDs) have generated considerable experimental and theoretical interest because of possible device applications. 1-7 In addition, they have highlighted the need to understand the fundamental physics involved in these and other quantum confined structures. A question which has attracted much attention and controversy concerns the time scales involved in the RTDs. In this work we focus attention on the dwell time (see later for a definition) which is perhaps the least controversial and the most well-accepted quantity. We study the dwell time and its first derivative with respect to position for both symmetric and asymmetric double barrier structures. These are physical quantities and can be obtained from stationary-state solutions of Schrödinger's equation. Since timedependent studies of Schrödinger's equation are computationally time consuming, our studies should provide qualitative guidelines in pursuing such studies. References 8-11 should provide the interested reader with some indications regarding the temporal aspects of resonance tunneling structures.

We consider an unbiased RTD with barrier heights V_i (i=1,2), barrier widths a_i (i=1,2) and electron effective masses in the barriers m_i^* (i=1,2) (in units of the free electron mass). The potential well has width d, and the effective mass inside the well and the contact regions are assumed to be m^* . Typically the barriers consist of $Al_{0.3}^{Ga}$ $O_{0.7}^{Ga}$ and the well consists of GaAS, so that $m_1^* = m_2^*$ $O_{0.09}$ and $m^* = 0.067$. The stationary-state properties of the resonant tunneling structure in the effective mass approximation are obtained by solving the time-independent Schrödinger's equation for the envelope function $\psi(z)$ along the growth direction z: 12

where V(z) is the conduction band potential energy profile, E is the incident energy, m is the electron mass, and a,b are constants. The importance of writing the kinetic energy term in a form similar to the first term of Eq. (la) was pointed out by Bastard. 13 The constants a and b in Eq. (1) must appear in the form given in order to make the Hamiltonian Hermitian. The above form of the kinetic energy operator is due to Morrow and Brownstein 12 and is a generalization of Bastard's form. At the heterojunction interfaces, which we have assumed to be abrupt, the kinetic energy operator dictates the matching conditions on $\psi(z)$ and its spatial derivative. We demand that $m \psi$ and $m^{(a+b)}(d\psi/dz)$ be continuous across an interface, implying the physical result that the current density $j \propto \psi^* (d\psi/dz)/m = m^2 \psi^*$ $m^{(a+b)}(d\psi/dz)$ be continuous. However, in general, the charge density $\rho \propto \psi * \psi$ need not be continuous across an interface. For the special case of a = 0 and b = -1 we obtain, in addition, the continuity of charge density.



	ssion For	
	GRA&I	
DTIC TAB		
Just	ification_	
	ibution/	
Dist	Avail and Special	/or
A-1		

/ 2

where, $x_i = (1/2)\delta_i \tanh \kappa_i a_i (i - 1, 2)$ with $\delta_i = [(m_i^*/m^*)^a \kappa_i/k - (m^*/m_i^*)^a k/\kappa_i]$ (i = 1,2), k =

 $(2m*E/N^2)^{\frac{1}{2}}$ and $\kappa_i = [2m_i^*(V_i - E)/N^2]^{\frac{1}{2}}$, (i = 1,2). For E > V_1 or V_2 , the hyperbolic functions should be replaced by appropriate circular functions, and κ_i should be imaginary. If the RTD is symmetric, with $V_1 - V_2 - V$, $a_1 - a_2$ and $m_1^* - m_2^* - m^*$, we recover Hauge et. al's result

(cot kd) =
$$-\frac{1}{2}(\kappa_1/k - k/\kappa_1) \tanh \kappa_1 a_1$$
 (3)

In Table 1 we show the lowest resonance energy of a symmetric (E_r) and an asymmetric (E_r^a) RTD as a function of the parameter b {Eq. (1)}.

Table 1. Dependence of the lowest resonance energy on the parameter b of Eq. (1). E_r and $E_{0.5}$ are, respectively, the resonance energy and energy for a transmission coefficient of 0.5 for a symmetric structure with $V_1 - V_2 - 200$ meV, d = 100 Å, $a_1 - a_2 = 50$ Å, $m^* = 0.067$ and $m_1^* - m_2^* = 0.09$. E_r^a is the resonance energy for an asymmetric double barrier with $V_1 = 100$ meV, $V_2 = 200$ meV, $d = a_1 - a_2 = 50$ Å, $m^* = 0.067$ and $m_1^* - m_2^* = 0.09$.

ь	E _r (meV)	E 0.5 (meV)	${\tt E}_{\tt r}^{\tt a}({\tt meV})$
-2	24.6738	24.6347	47.9598
-1	28.8350	28.7975	57.3208
0	32.9650	32,9300	66.9193
1	36,8850	36.8567	76.1235
2	40,4560	40.4337	84.1560

The resonance energy clearly depends on the parameter b; we cannot, a priori, prefer one value of b over another. We study below the dependence of other physical quantities on the

parameter b. The dwell time $\tau_{\rm D}$ over the region 0 to $z_{\rm l}$ of the structure is defined 7,15 as the integrated probability density of the electron divided by the incident flux:

$$\tau_{\rm D} = \int_0^{z_1} dz |\psi(z)|^2 /(k/m^*)$$
 (4)

The associated average local speed v at a given point z in the structure is

$$v^{-1} - \partial \tau_D / \partial z \quad . \tag{5}$$

We have studied the dwell times and average local speeds of an electron in a double barrier structure for energies in the neighborhood of the resonance energy E_r . Figures 1-3 show r_n and v^{-1} for two energies E_r (transmission coefficient T = 1) and $E_{0.5}$ (T = 0.5) as a function of the parameter b. These figures clearly show wide variations in the magnitudes of the above physical quantities as one changes b. The discontinuities in the velocities (as long as b is not equal to -1) at the two interfaces arise from the discontinuities of charge at the interfaces, as already mentioned. Note also that the discontinuities could be positive or negative at a given interface. The behavior of $r_{\rm D}$ and v^{-1} for an asymmetric structure are similar (Figs. 4-6); however, the discontinuities of v⁻¹ are more prominent in this case.

We have thus shown that the parameter associated with matching condition at the interfaces has a profound effect on the characteristics of the system such as resonance energy, dwell time and the average local speed. It has been shown, \$16,17\$ in a different context, that for two semi-finite heterostructures, the matching conditions at the interface not only involve the effective masses but also certain other parameters which are microscopic in origin, having no macroscopic analogs. We therefore believe that the arbitrariness in the choice of the parameter b [Eq. (1)] above can

be fixed through microscopic calculations.

Acknowledgment - This work was supported in part by the Office of Naval Research and the Air Force Office of Scientific Research (AFSC), United States Air Force, under Contract F49620-86-C-0009.

References

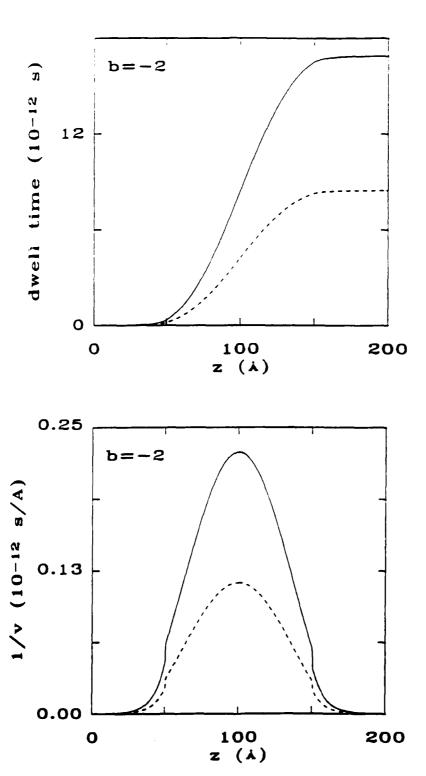
- 1. L. L. Chang, L. Esaki and R. Tsu, Applied Physics Letters 24, 593 (1974).
- T. C. L. G. Sollner, W. D. Goodhue, P. E. Tannenwald, C. D. Parker and D. D. Peck, Applied Physics Letters 43, 588 (1983).
- 3. E. T. Yu and T. C. McGill, Applied Physics Letters 53, 60 (1988).
- 4. A. Zaslavsky, V. J. Goodman, D. C. Tsui and J. E. Cunningham, Applied Physics Letters 53, 1408 (1988).
- 5. B. Ricco and M. Ya. Azbel, Physical Review B 29, 1970 (1984).
- E. H. Hauge, J. P. Falck and T. A. Fjeldly, Physical Review B, 36, 4203 (1987).
- 7. C. R. Leavens and G. C. Aers, Physical Review B 39, 1202 (1989) and preprint.
- 8. F. Ancilotto, A. Selloni, L. F. Xu and E. Tosatti, Physical Review B, 39, 8322 (1989).
- 9. S. Collins, D. Lowe and J. R. Barker, Journal of Physics C <u>20</u>, 6233 (1987).
- 10. A. P. Jauho and M. M. Nieto, Superlattices and Microstructures 2, 407 (1986).
- 11. M. C. Yalabik, G. Noefatosto, K. Diff, H. Guo and J. D. Guntow, IEEE Transactions on Electron Devices 36, 1009 (1989).
- 12. R. A. Morrow and K. R. Brownstein, Physical Review B 30, 678 (1984).
- 13. G. Bastard, PhysicalReview B <u>24</u>, 5693 (1981).
- 14. Following Ref. 6, we have derived Eq. (2) from the condition dT/d'd' = 0, where T is the square of the transmission amplitude and 'd' is the well width. Conventionally, the resonance condition is obtained from dT/dE = 0. For a symmetric structure, the two definitions are equivalent. For an asymmetric structure, the direction along which the derivative is evaluated makes a difference; it is believed, however, that the difference between the two is exponentially small.

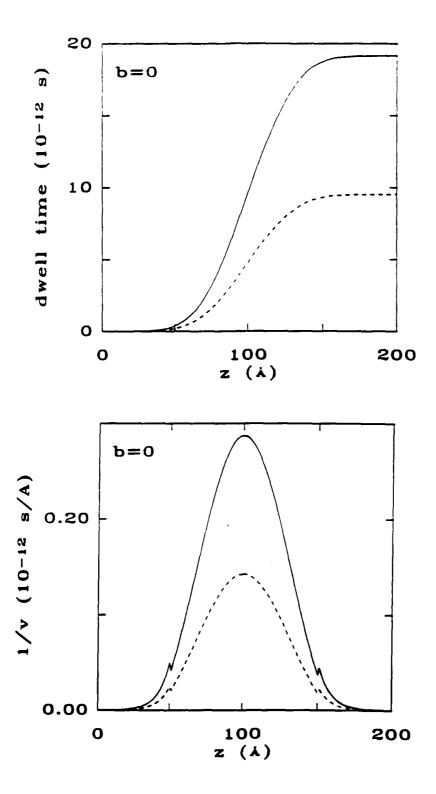
- 15. M. Büttiker, Physical Revie B <u>27</u>, 6178 (1983).
- 16. W. Trzeciakowski, Physical Review B 38, 4322 (1988).
- 17. A. A. Grinberg and S. Luryi, Physical Review B 39, 7466 (1989).

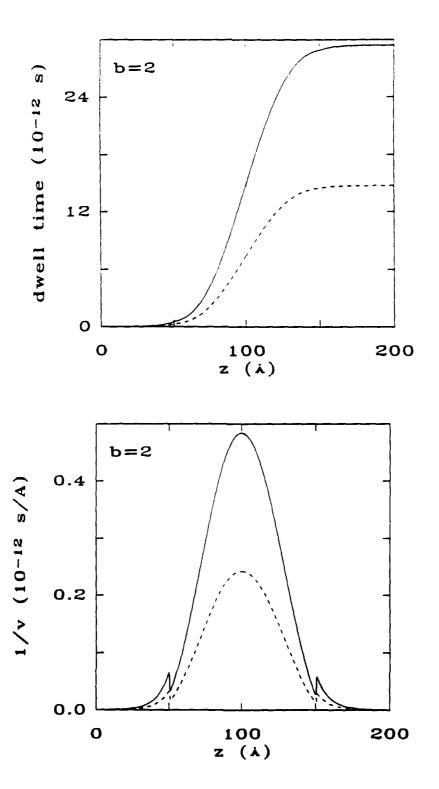
Figure Captions

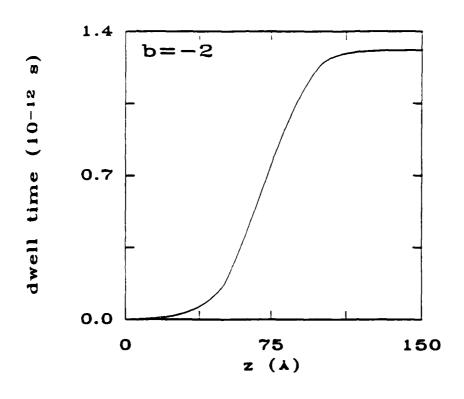
- Fig. 1. Dwell time (top panel) and inverse of the average local speed (bottom panel) as a function of position z relative to left most edge of the structure. The parameters are: b = $^{-2}$, V 1 = V 2 = 200 0 meV, d 4 = 100 Å, a 1 = a 2 = 50 Å, m 4 = $^{0.067}$ and m 1 = m 2 = $^{0.09}$. The solid line corresponds to resonance and the dashed line to a transmission coefficient of $^{0.5}$.
- Fig. 2. Dwell time (top panel) and inverse of the average local speed (bottom panel) as a function of position z relative to leftmost edge of the structure. The parameters are: b = 0, $V_4 V_2 200$ meV, $d_* 100$ Å, $d_* d_* 50$ Å, $d_* 0.067$ and $d_* d_* 0.09$. The solid line corresponds to resonance and the dashed line to a transmission coefficient of 0.5.
- Fig. 3. Dwell time (top panel) and inverse of the average local speed (bottom panel) as a function of position z relative to leftmost edge of the structure. The parameters are: b = 2, $V_4 = V_2 = 200$ meV, $d_* = 100$ Å, $d_* = d_* = 50$ Å, $d_* = 0.067$ and $d_* = d_* = 0.09$. The solid line corresponds to resonance and the dashed line to a transmission coefficient of 0.5.
- Fig. 4. Dwell time (top panel) and inverse of the average local speed (bottom panel) as a function of position z relative to the edge of the smaller of the two asymmetric barriers. The parameters are: b = -2, $V_{\pm} = 100$ meV, $V_{\pm} = 200$ meV, $d = a_1 = a_2 = 50$ Å, $m^{\pm} = 0.067$ and $m_1 = m_2 = 0.09$.
- Fig. 5. Dwell time (top panel) and inverse of the average local speed (bottom panel) as a function of position z relative to the edge of the smaller of the two asymmetric barriers. The parameters are: b = 1, $V_1 = 100$ meV, $V_2 = 200$ meV, $d = a_1 = a_2 = 50$ Å, m = 0.067 and $m_1 = m_2 = 0.09$.
- Fig. 6. Dwell time (top panel) and inverse of the average local speed (bottom panel) as a function of position z relative to the edge of the smaller of the two asymmetric barriers.

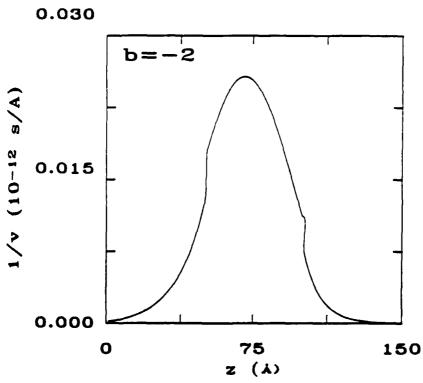
The parameters are: b = 2, $v_1 = 100$ meV, $v_2 = 200$ meV, $c = a_1 = a_2 = 50$ Å, c = 0.067 and c = 0.091.

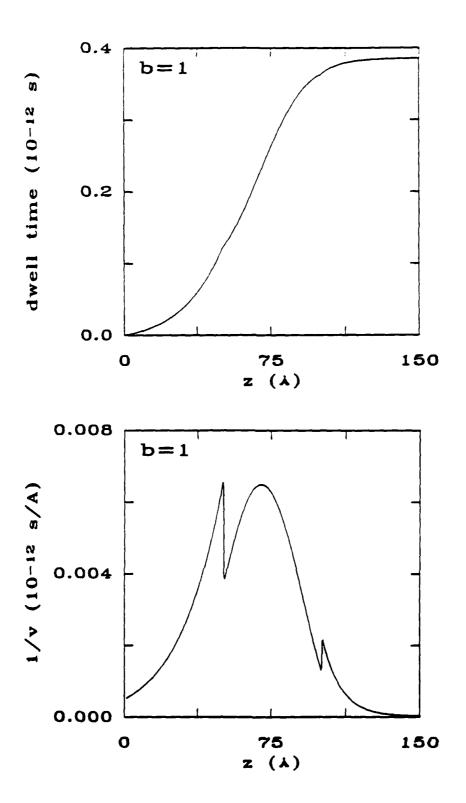


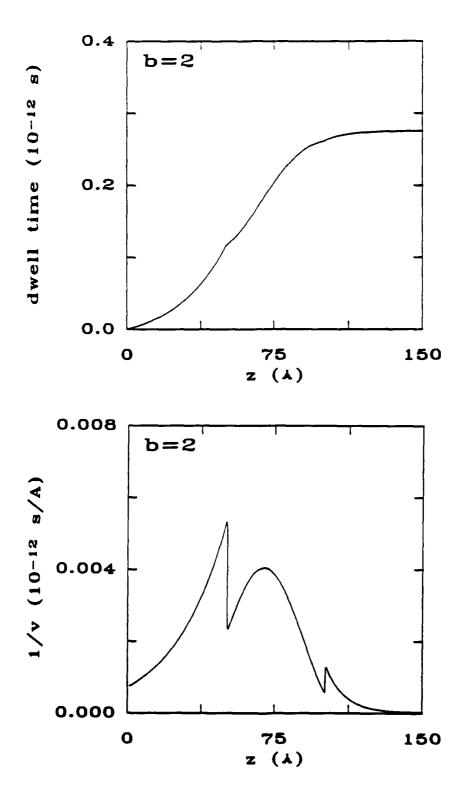












01/1113/86/2

TECHNICAL REPORT DISTRIBUTION LIST, GEN

	No. Copies	•	No. Copies
Office of Naval Research Attn: Code 1113 800 N. Quincy Street Arlington, Virginia 22217-5000	2	Dr. David Young Code 334 NORDA NSTL, Mississippi 39529	1
Or. Bernard Douda Naval Weapons Support Center Code 50C Crane, Indiana 47522-5050	1	Naval Weapons Center Attn: Dr. Ron Atkins Chemistry Division China Lake, California 93555	1
Naval Civil Engineering Laboratory Attn: Dr. R. W. Drisko, Code L52 Port Hueneme, California 93401	1	Scientific Advisor Commandant of the Marine Corps Code RD-1 Washington, D.C. 20380	1
Defense Technical Information Center Building 5, Cameron Station Alexandria, Virginia 22314	12 high quality	U.S. Army Research Office Attn: CRD-AA-IP P.O. Box 12211 Research Triangle Park, NC 27709	1
DTNSRDC Attn: Dr. H. Singerman Applied Chemistry Division Annapolis, Maryland 21401	1	Mr. John Boyle Materials Branch Naval Ship Engineering Center Philadelphia, Pennsylvania 19112	
Dr. William Tolles Superintendent Chemistry Division, Code 6100 Naval Research Laboratory	1	Naval Ocean Systems Center Attn: Dr. S. Yamamoto Marine Sciences Division San Diego, California 91232	1
Washington, D.C. 20375-5000		Dr. David L. Nelson Chemistry Division Office of Naval Research 800 North Quincy Street Arlington, Virginia 22217	1

Dr. J. E. Jensen Hughes Research Laboratory 3011 Malibu Canyon Road Malibu, California 90265

Dr. J. H. Weaver
Department of Chemical Engineering
and Materials Science
University of Minnesota
Minneapolis, Minnesota 55455

Dr. A. Reisman
Microelectronics Center of North Carolina
Research Triangle Park, North Carolina
Chemistry Depa
27709
George Washing

Dr. M. Grunze
Laboratory for Surface Science and
Technology
University of Maine
Orono, Maine 04469

Dr. J. Butler Naval Research Laboratory Code 6115 Washington D.C. 20375-5000

Dr. L. Interante Chemistry Department Rensselaer Polytechnic Institute Troy, New York 12181

Dr. Irvin Heard Chemistry and Physics Department Lincoln University Lincoln University, Pennsylvania 19352

Dr. K.J. Klaubunde Department of Chemistry Kansas State University Manhattan, Kansas 66506 Dr. C. B. Harris
Department of Chemistry
University of California
Berkeley, California 94720

Dr. F. Kutzler
Department of Chemistry
Box 5055
Tennessee Technological University
Cookesville, Tennessee 38501

Dr. D. Dilella Chemistry Department George Washington University Washington D.C. 20052

Dr. R. Reeves Chemistry Department Renssaeler Polytechnic Institute Troy, New York 12181

Dr. Steven M. George Stanford University Department of Chemistry Stanford, CA 94305

Dr. Mark Johnson Yale University Department of Chemistry New Haven, CT 06511-8118

Dr. W. Knauer Hughes Research Laboratory 3011 Malibu Canyon Road Malibu, California 90265

Dr. G. A. Somorjai Department of Chemistry University of California Berkeley, California 94720

Or. J. Murday Naval Research Laboratory Code 6170 Washington, D.C. 20375-5000

Dr. J. B. Hudson Materials Division Rensselaer Polytechnic Institute Troy, New York 12181

Dr. Theodore E. Madey Surface Chemistry Section Department of Commerce National Bureau of Standards Washington, D.C. 20234

Dr. J. E. Demuth
IBM Corporation
Thomas J. Watson Research Center
P.O. Box 218
Yorktown Heights, New York 10598

Dr. M. G. Lagally
Department of Metallurgical
and Mining Engineering
University of Wisconsin
Madison, Wisconsin 53706

Or. R. P. Van Duyne Chemistry Department Northwestern University Evanston, Illinois 60637

Dr. J. M. White Department of Chemistry University of Texas Austin, Texas 78712

Or. O. E. Harrison Department of Physics Naval Postgraduate School Monterey, California 93940 Or. R. L. Park
Director, Center of Materials
Research
University of Maryland
College Park, Maryland 20742

Dr. W. T. Peria Electrical Engineering Department University of Minnesota Minneapolis, Minnesota 55455

Dr. Keith H. Johnson
Department of Metallurgy and
Materials Science
Massachusetts Institute of Technology
Cambridge, Massachusetts 02139

Dr. S. Sibener
Department of Chemistry
James Franck Institute
5640 Ellis Avenue
Chicago, Illinois 60637

Anceld
Dr. Amnold Green
Quantum Surface Dynamics Branch
Code 3817
Naval Weapons Center
China Lake, California 93555

Dr. A. Wold Department of Chemistry Brown University Providence, Rhode Island 02912

Dr. S. L. Bernasek Department of Chemistry Princeton University Princeton, New Jersey 08544

Dr. W. Kohn
Department of Physics
University of California, San Diego
La Jolla, California 92037

Dr. F. Carter Code 6170 Naval Research Laboratory Washington, D.C. 20375-5000

Dr. Richard Colton Code 6170 Naval Research Laboratory Washington, D.C. 20375-5000

Dr. Dan Pierce National Bureau of Standards Optical Physics Division Washington, D.C. 20234

Dr. R. Stanley Williams
Department of Chemistry
University of California
Los Angeles, California 90024

Dr. R. P. Messmer Materials Characterization Lab. General Electric Company Schenectady, New York 22217

Dr. Robert Gomer Department of Chemistry James Franck Institute 5640 Ellis Avenue Chicago, Illinois 60637

Dr. Ronald Lee R301 Naval Surface Weapons Center White Oak Silver Spring, Maryland 20910

Dr. Paul Schoen Code 6190 Naval Research Laboratory Washington, D.C. 20375-5000 Dr. John T. Yates Department of Chemistry University of Pittsburgh Pittsburgh, Pennsylvania 15260

Dr. Richard Greene Code 5230 Naval Research Laboratory Washington, D.C. 20375-5000

Dr. L. Kesmodel
Department of Physics
Indiana University
Bloomington, Indiana 47403

Dr. K. C. Janda University of Pittsburg Chemistry Building Pittsburg, PA 15260

Dr. E. A. Irene Department of Chemistry University of North Carolina Chapel Hill, North Carolina 27514

Dr. Adam Heller Bell Laboratories Murray Hill, New Jersey 07974

Dr. Martin Fleischmann Department of Chemistry University of Southampton Southampton 509 5NH UNITED KINGDOM

Dr. H. Tachikawa Chemistry Department Jackson State University Jackson, Mississippi 39217

Dr. John W. Wilkins Cornell University Laboratory of Atomic and Solid State Physics Ithaca, New York 14853

Dr. R. G. Wallis Department of Physics University of California Irvine, California 92664

Dr. D. Ramaker Chemistry Department George Washington University Washington, D.C. 20052

Dr. J. C. Hemminger Chemistry Department University of California Irvine, California 92717

Dr. T. F. George Chemistry Department University of Rochester Rochester, New York 14627

Dr. G. Rubloff IBM Thomas J. Watson Research Center P.O. Box 218 Yorktown Heights, New York 10598

Dr. Horia Metiu Chemistry Department University of California Santa Barbara, California 93106

Dr. W. Goddard
Department of Chemistry and Chemical
Engineering
California Institute of Technology
Pasadena, California 91125

Or. P. Hansma
Department of Physics
University of California
Santa Barbara. California 93106

Dr. J. Baldeschwieler
Department of Chemistry and
Chemical Engineering
California Institute of Technology
Pasadena, California 91125

Dr. J. T. Keiser Department of Chemistry University of Richmond Richmond, Virginia 23173

Or. R. W. Plummer Department of Physics University of Pennsylvania Philadelphia, Pennsylvania 19104

Dr. E. Yeager Department of Chemistry Case Western Reserve University Cleveland, Ohio 41106

Dr. N. Winograd
Department of Chemistry
Pennsylvania State University
University Park, Pennsylvania 16802

Dr. Roald Hoffmann Department of Chemistry Cornell University Ithaca, New York 14853

Dr. A. Steckl
Department of Electrical and
Systems Engineering
Rensselaer Polytechnic Institute
Troy, NewYork 12181

Dr. G.H. Morrison Department of Chemistry Cornell University Ithaca, New York 14853